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EXAMINER	
DEJONG, ERIC S	

ART UNIT	PAPER NUMBER
1631	

DATE MAILED: 03/16/2006

Please find below and/or attached an Office communication concerning this application or proceeding.

Office Action Summary	Application No.	Applicant(s)	
	09/506,717	HELSON, HAROLD E	
	Examiner	Art Unit	
	Eric S. DeJong	1631	

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

1)☒ Responsive to communication(s) filed on *12/16/2005*.

2a)☒ This action is **FINAL**. 2b)☐ This action is non-final.

3)☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

4)☒ Claim(s) *5-16 and 19-27* is/are pending in the application.

4a) Of the above claim(s) _____ is/are withdrawn from consideration.

5)☐ Claim(s) _____ is/are allowed.

6)☒ Claim(s) *5-16 and 19-27* is/are rejected.

7)☐ Claim(s) _____ is/are objected to.

8)☐ Claim(s) _____ are subject to restriction and/or election requirement.

Application Papers

9)☐ The specification is objected to by the Examiner.

10)☐ The drawing(s) filed on _____ is/are: a)☐ accepted or b)☐ objected to by the Examiner.

Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).

Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).

11)☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

Priority under 35 U.S.C. § 119

12)☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).

a)☐ All b)☐ Some * c)☐ None of:

1.☐ Certified copies of the priority documents have been received.

2.☐ Certified copies of the priority documents have been received in Application No. _____.

3.☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

* See the attached detailed Office action for a list of the certified copies not received.

Attachment(s)

1) ☐ Notice of References Cited (PTO-892)
2) ☐ Notice of Draftsperson's Patent Drawing Review (PTO-948)
3) ☐ Information Disclosure Statement(s) (PTO-1449 or PTO/SB/08) Paper No(s)/Mail Date _____.
4) ☐ Interview Summary (PTO-413) Paper No(s)/Mail Date. _____ .
5) ☐ Notice of Informal Patent Application (PTO-152)
6) ☐ Other: _____.

DETAILED OFFICE ACTION

SUBSTANTIAL CLAIM DUPLICATION

Applicant is advised that should claims 7 and 8 be found allowable, claims 7 and 8 will be objected to under 37 CFR 1.75 as being a substantial duplicate thereof. When two claims in an application are duplicates or else are so close in content that they both cover the same thing, despite a slight difference in wording, it is proper after allowing one claim to object to the other as being a substantial duplicate of the allowed claim. See MPEP § 706.03(k).

Claim Rejections - 35 USC § 112, First Paragraph

The following is a quotation of the first paragraph of 35 U.S.C. 112:

> The specification shall contain a written description of the invention, and of the manner and process of making and using it, in such full, clear, concise, and exact terms as to enable any person skilled in the art to which it pertains, or with which it is most nearly connected, to make and use the same and shall set forth the best mode contemplated by the inventor of carrying out his invention.

Claims 22-27 are rejected under 35 U.S.C. 112, first paragraph, as failing to comply with the written description requirement. The claim(s) contains subject matter which was not described in the specification in such a way as to reasonably convey to one skilled in the relevant art that the inventor(s), at the time the application was filed, had possession of the claimed invention. This rejection is newly applied and necessitated by amendment.

Claims 22-27 each recite the limitation of drawn to "tracing a path through the structure, assigning bond orders and atomic charges/radicals as the path is traced, and

backtracking the path when an inconsistency is detected." However, upon review of the instant disclosure, no direct or specific support has been found the above specified limitation. Page 5, lines 8-12 of the instant specification states:

"Conceptually, in a specific embodiment of the procedure, a path is traced through the structure and, for each atom, each possible electronic and bonding state is examined that is consistent with the previous results along the path. By extensively or exhaustively examining possible states and orders, the procedure is able to arrive at a fixed bond solution, if one exists."

It is noted that this portion of the specification generally describes tracing a path through the structure and for each atom examining each possible electronic and binding state. However, this portion of the specification is silent in regards to assigning bond orders and atomic charges/radicals as the path is traced. Further, this portion of the specification is silent as to backtracking the path when an inconsistency is found.

Page 11, lines 1-2 provides for a general procedure illustrated in Figs. 10 and 22, which is further describes through page 11, lines 2 through page 13, line 2. The general procedure described in Fig. 22 provides for the following steps (letters and numbers delineating the steps have been added for clarity):

(A) Select an initial atom;
(B) Assign a bond order to an adjacent bond,
(C) Assign, to a next adjacent atom, an ESVD that is consistent with the previous bond;
(D) Select the next adjacent atom, and ESVD that is consistent with the previous bond;
(E) Repeat the same approach for additional atoms;
(F) If an unacceptable state is encountered
    (i) Reject the path values
    (ii) Backtrack to the last point where a selection was made and proceed forward from there with a different selection;
(G) If a solution is found that cannot be improved upon, terminate;
(H) If a solution is found that is not optimal and there are other choices, explore the other choices

The general procedure described above is more narrowly defined than broader limitation that is instantly claimed. Steps (B) and (C) are specific in that bond orders and an ESVD are assigned between adjacent atoms. The instant claim generically recites assigning bond order and atomic charge as the path is traced, and does not recite a limitation drawn to assigning an ESVD. Step (F) is specific in that it involves backtracking to the last point where a selection was made when an unacceptable state is encountered. Further, steps (G) and (H) that are drawn to solutions that cannot be improved upon and solutions that are not optimal, respectively. In contrast, the instant claims do not specify the position in the traced path that the backtracking falls back to and generically recites backtracking when an inconsistency is detected. The specification does not provide a definition for the claimed term of "inconsistency" nor does it provide a teaching wherein an "inconsistency" is equated to "an unacceptable state" or solutions that are "not optimal" or "cannot be improved upon".

While the instant disclosure provides for the more narrow embodiments described above, the specification does not provide sufficient support that is commensurate in scope with the more broad claimed limitation "tracing a path through the structure, assigning bond orders and atomic charges/radicals as the path is traced, and backtracking the path when an inconsistency is detected." Therefore, said limitation is regarded as NEW MATTER.

Claim Rejections - 35 USC § 102(a)

The following is a quotation of the appropriate paragraphs of 35 U.S.C. 102 that form the basis for the rejections under this section made in this Office action:

> A person shall be entitled to a patent unless –
>
> (a) the invention was known or used by others in this country, or patented or described in a printed publication in this or a foreign country, before the invention thereof by the applicant for a patent.

Claims 5-16 and 19-21 are rejected under 35 U.S.C. 102(a) as being anticipated by Glendening et al.

The pending claims are drawn to methods and related computer systems and software for use in deriving fixed bond information from a delocalized structure representation. The claimed invention comprises the steps of analyzing a delocalized representation of a chemical structure that contains at least in part a polycyclic ring system, identifying a plurality of fixed bond representations candidates based on valence information, evaluating a subset of the fixed bond representations, selecting fixed bond representation candidates based on the evaluation, producing fixed bond information based on the selection and outputting said fixed bond information.

[Claims 5, 19, 20, and 21]: Glendening et al. sets forth a quantum-mechanical resonance theory based on a first-order reduced density matrix and a representation of chemical structures in terms of natural bond orbitals. A "natural" resonance theory is disclosed that leads to an optimal resonance-weighted approximation to the full density matrix, wherein the "single reference" limit of weak delocalization is combined with full "multireference" limit of strong delocalization. The results provide an intrinsic criterion of accuracy of the resonance-theoretic description. See Glendening et al., Abstract.

Glendening et al. sets forward an analysis program that takes as input a resonance structure and performs a quasi-quantum mechanical analysis on delocalized structures to establish natural bond orders (NBO) for formalized Lewis structures which read on the limitation of producing and outputting fixed bond information in a selected fixed bond structure. See Glendening et al., page 597, column 1, lines 15-39. The conceptual methodology employed in the algorithm rely on valence theory in establishing resultant fixed bond structure. See Glendening et al., page 597, lines 34-39. The disclosed methodology and system provides for the generation of several possible structures from a starting resonance or delocalized chemical input structure and a selection routine to pick from the generated structures the most plausible fixed structure candidate. See Glendening et al., page 602, column 2, line 13 through, page 604, column 1, line 29. The program is fully capable of accepting polycyclic structures as demonstrated on page 603, column 2, line 34 through page 604, column 1, line 3.

[Claim 6]: The disclosed methodology explicitly accounts for molecular situations where delocalization effects are so strong that no NBO Lewis structure is dominant. This is broadly construed as reading on a delocalized chemical representation with a hetero-substitution pattern. See Glendening et al., page 600, column 1, line 6 through column 2, line 8.

[Claims 7 and 8]: Specific examples are provided wherein the methodology is capable of accepting and operating on portions of delocalized chemical representation that describe a non-cyclic/acyclic system. See for example Glendening et al., page 594, column 1, line 17 through column 2, line12. For the purposes of examination, the

limitations of a non-cyclic system and acyclic system are both construed as chemical systems that do consist of a cyclical chemical structure.

[Claims 9 and 10]:The methodology set forth by Glendening et al. also accounts or producing fixed bond structures that include a pair of opposite charges as well as a pair of radicals that are lacked by the delocalized representation. See for example Glendening et al., page 597, column 2, lines 1-27.

[Claims 11 and 15]: The instant specification on page 6, lines 10-13, is relied upon for possible definition of an ESVD as the collection of characteristics pertaining to an atomic environment such as charge, any unpaired electrons, and bonding information. As such, Glendening et al. a delocalization list of NBO interactions of a parent reference structure used to generate a list of the associated secondary structures describing a delocalized hybrid. Given the formal resonance structures, the NBO program is able to calculate the optimal set of NBOs for a given structure. Under a reasonably broad interpretation these teaching read on the claimed limitation of identifying based on an ESVD as well as queing at least a subset of the ESVDs by priority.

[12-14]: Glendening et al. sets forth the use of the NRT program for sampling a wide variety of candidate structures. Said structures can be generated from several alternatives such as the Wiberg bond index, the delocalization lists for any previous list of candidate structures, or specified by the user of the program. See Glendening et al., page 598, column 1, line 38 through column 2, line 7. As such, under a reasonably broad interpretation, the disclosed methodology and systems read on the claimed

limitation of using a pre-computed table. The alternatives presented by Glendening et al. also cover allowing additional elements and values to be added to the table as well as additions being applied to any chemical element.

[Claim 16]: The disclosed practicality of the NRT method is indicated by the computation time used to arrive at a particular or given set of structures. The methods and systems set forth in Glendening et al. are customizable so that either a set number of iterations are performed, thus providing a selectable longer or shorter set of expanded structures generated by the program. See Glendening et al., page 608, column 1, lines 1-36.

Claim Rejections - 35 USC § 102(b)

The rejection of claim 5, 11, 15, and 20 under 35 USC § 102(b) as being anticipated by Garaovac et al. is withdrawn in view of amendments made to the instant claims and arguments presented by applicants.

Claim Rejections - 35 USC § 103

The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all obviousness rejections set forth in this Office action:

> (a) A patent may not be obtained though the invention is not identically disclosed or described as set forth in section 102 of this title, if the differences between the subject matter sought to be patented and the prior art are such that the subject matter as a whole would have been obvious at the time the invention was made to a person having ordinary skill in the art to which said subject matter pertains. Patentability shall not be negatived by the manner in which the invention was made.

Claims 5, 11, 15, and 20 are rejected under 35 U.S.C. 103(a) as being unpatentable over Graovac et al. This rejection is necessitated by amendments made to the instant claims.

The pending claims are drawn to methods and related computer systems and software for use in deriving fixed bond information from a delocalized structure representation. The claimed invention comprises the steps of analyzing a delocalized representation of a chemical structure that contains at least in part a polycyclic ring system, identifying a plurality of fixed bond representations candidates based on valence information, evaluating a subset of the fixed bond representations, selecting fixed bond representation candidates based on the evaluation, producing fixed bond information based on the selection and outputting said fixed bond information.

In Graovac et al. the abstract summarizes the description therein as being directed to utilizing valence structures of hydrocarbon systems to produce a Kekule index which corresponds to Kekule-type valence structures. These structures are evaluated via the empirical Fries rule to predict stability. Table I on page 6269 lists various Kekule structures which have been identified and evaluated via Kekule indices which are deemed to be practices as in lines 2-5 of instant claim 5. The indices are also deemed to be fixed bond information as required in the instant claims, such as in claim 5, line 8. Specific fixed bond structures are selected, as well as discussed, from said Table I on page 6269, right-hand column, lines 4-40, which anticipates selecting practice as in instant claim 5, lines 6-7. The ring system structures in said Table I are clearly polycyclic ring systems as required in instant claim 5, last 2 lines. These

structures also depict the electronic state and valence distribution information via the bonding as required in instant claim 15. The reference also sets forth a system as in instant claim 20 as the reference is directed to a methodology system reasonably as in instant claim 20 which lacks any specific limitations which specify a system therein to exclude such a methodology system as in the reference. Several fixed bond structures in Table I-III (page 6270) are lined up with the highest Kekule index as the left most structure with decreasing index to the right. See, for example, Table I, second row of structures directed to phenanthrene wherein the index goes from 0.913 (0.931) to 0.897 (0.890) which is a type of priority queuing as required in instant claim 11. Thus, these descriptions in Graovac et al. anticipate the above listed instant claims.

Graovac et al. sets forth the above described methods and related systems deriving fixed bond information from a delocalized structure representation, which reads on the process steps recited in the instant claims. However, Graovac et al. does not fairly teach or disclose a computer readable medium holding computer readable code for the disclosed method steps.

Regarding computer-related invention, the MPEP §2106(VI) states:

As is the case for inventions in any field of technology, assessment of a claimed computer-related invention for compliance with 35 U.S.C. 102 and 103 begins with a comparison of the claimed subject matter to what is known in the prior art. If no differences are found between the claimed invention and the prior art, the claimed invention lacks novelty and is to be rejected by Office personnel under 35 U.S.C. 102. Once distinctions are identified between the claimed invention and the prior art, those distinctions must be assessed and resolved in light of the knowledge possessed by a person of ordinary skill in the art. Against this backdrop, one must determine whether the invention would have been obvious at the time the invention was made. If not, the claimed invention satisfies 35 U.S.C. 103. Factors and considerations dictated by law governing 35 U.S.C. 103 apply without modification to computer-related inventions. Moreover, merely using a computer to automate a known process does not by itself impart nonobviousness to the invention. See In re Venner, 262 F.2d 91, 95, 120 USPQ 193, 194 (CCPA 1958). See also Dann v. Johnston, 425 U.S. 219, 227-30, 189 USPQ 257, 261 (1976).

Therefore, it would have been obvious at the time the invention was made to a person having ordinary skill in the art to which said subject matter pertains to automate the disclosed methods for deriving fixed bond information from a delocalized structure representation using computer readable medium holding computer readable code, since reliance on a computer to automate a known process does not by itself impart nonobviousness.

Response to Arguments

Applicant's arguments filed 12/16/2005 have been fully considered but they are not persuasive.

In regards to the rejection of claims 5-16 and 19-21 under 35 USC 102(a) as being anticipated by Glendening et al., applicants argue that the reference does not disclose or suggest analyzing a delocalized representation of a chemical structure, wherein said representation comprises a two-dimensional structure drawing. Applicants

refer to page 602 of Glendening et al. under the heading of "Generation of Resonance Structures" that discloses given wave function ψ, the NRT program constructs a list of one or more parent "reference" Lewis structures that describe the leading delocalization in the molecule". On this basis, applicants argue that Glendening therefore does not analyze a delocalized representation of a chemical structure wherein said representation comprises a two-dimensional structure drawing.

In response to applicant's argument, it is noted that amended claim 5 now recites "said representation comprises a two-dimensional structure drawing." As such, the limitation is drawn to analyzing a delocalized representation comprising any two-dimensional structure drawing and is not limited to drawings of delocalized structure. As acknowledged by applicants, the method and systems disclosed by Glendening et al. does analyze a delocalized representation of a chemical structure by a given wave function ψ and the program routine LEWIS returns reference chemical structures (see also the polycyclic chemical structures presented on page 603 col. 2, of Glendening et al.), which anticipates the claimed limitation drawn to analyzing a delocalized representation of a chemical structure wherein said representation comprises a two-dimensional structure drawing. Therefore applicants argument is not found persuasive.

Applicants further argue that Glendening et al. does not disclose or suggest identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure. Applicants refer to Glendening et al., page 597, col. 1, lines 34-39 and argue the reference does not

disclose how resonance structures are enumerated but only states that the structures are in agreement with elementary valence theory.

In response, it is noted that the instant claim 5 recites in lines 6 and 7 the limitation of "identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure." This limitation is broad in that is does not expressly limit how the step of identifying candidates is to be performed using valence information. Further, the claimed limitation does not limit or specify the type of valence information relied upon in the identification step. In the instant case, the valance information relied upon by Glendening et al. is that the Lewis structures generated by the disclosed method are consistent with elementary valence theory. As such, valence information is relied upon in the generation of Lewis structures and properly reads on the claimed limitation. Therefore applicants arguments are not found persuasive.

Applicant's argument that Graovac et al. does not disclose or suggest a computer-implemented method is considered moot in view of the new ground of rejection presented above.

In regards to Graovac et al., applicants argue that Graovac et al. does not disclose a delocalized structure representation. Applicants further argue that even if the Figs. 1 and 2 can be said to disclose delocalized structures, there is nothing in the reference to indicate that they are converted to fixed bond structures.

In response, it is noted that page 1, lines 10-16 states:

> "Since a well known chemist named Auguste Kekule suggested that double bonds were not fixed or localized, and depicted a benzene ring with a delocalizing circle instead of alternating single and double bonds, the process (i.e., cyclic delocalization) from a fixed-bond representation may be called "Kekulization." A Kekule structure representation is one in which the alternating single and double bonds of the classical depiction are replaced by all single bonds, adorned by a circle or arc."

By the teaching provided in the instant disclosure, it Kekule structures themselves are arrived at by implementing a process of delocalization. Therefore, the Kekule structures from Figs. 1 and 2 of Graovac et al. read on a delocalized representation of a chemical structure. Further, the Tables I-III of Graovac et al. read on fixed bond structures. It is also noted that the claims do not recite any limitation drawn to a "delocalized structure converted to a fixed bond structure." Rather, the instant claims recite the limitations drawn to producing fixed bond information and outputting the fixed bond information (see for example lines 11 and 12). As such, the recited limitation of "fixed bond information" is not limited to a converted fixed bond structure.

In regards to the rejection of claim 11, applicants further argue that the claimed step of queuing at least a subset of the ESVDs by priority is not disclosed or suggested by Graovac et al. Applicants specifically argue that Graovac et al. computes a property value for each structure which is a sorting process and not priority queuing.

In response to applicant's argument, it is noted that page 6, lines 11-13 teaches that an electronic state and valence distribution (ESVD) may include bonding information for an atomic environment. As such, the Kekule index for the sorted structures presented by Graovac et al. reads on a subset of ESVDs. Further, the instant claim is does not limit how these subset of ESVDs may be queued. As such, the fixed

bond structures in Table I-III (page 6270) lined up with the highest Kekule index as the left most structure with decreasing index to the right read on a priority queuing, wherein priority is demonstrated by the structures listed in ascending Kekule value.

Conclusion

Applicant's amendment necessitated the new ground(s) of rejection presented in this Office action. Accordingly, **THIS ACTION IS MADE FINAL**. See MPEP § 706.07(a). Applicant is reminded of the extension of time policy as set forth in 37 CFR 1.136(a).

A shortened statutory period for reply to this final action is set to expire THREE MONTHS from the mailing date of this action. In the event a first reply is filed within TWO MONTHS of the mailing date of this final action and the advisory action is not mailed until after the end of the THREE-MONTH shortened statutory period, then the shortened statutory period will expire on the date the advisory action is mailed, and any extension fee pursuant to 37 CFR 1.136(a) will be calculated from the mailing date of the advisory action. In no event, however, will the statutory period for reply expire later than SIX MONTHS from the date of this final action.

Any inquiry of a general nature or relating to the status of this application should be directed to Legal Instrument Examiner, Tina Plunkett, whose telephone number is (571) 272-0549.

Any inquiry concerning this communication or earlier communications from the examiner should be directed to Eric S. DeJong whose telephone number is (571) 272-6099. The examiner can normally be reached on 8:30AM-5:00PM.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Ardin Marschel, Ph.D. can be reached on (571) 272-0718. The fax phone number for the organization where this application or proceeding is assigned is (571) 273-8300.

Information regarding the status of an application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information about the PAIR system, see http://pair-direct.uspto.gov. Should you have questions on access to the Private PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free).

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EDJ EDJ

10 March 2000

JOHN S. BRUSCA, PH.D
PRIMARY EXAMINER